AWE

Science Engineering Technology at AWE

Discovery23

July 2012

This issue:

Reliable nuclear data are an essential component of the physics based modelling of neutronic systems. The principal responsibility of the Nuclear Data Team is to provide data suitable for use with AWE's modelling codes.

The term nuclear data, although associated with any intrinsic properties of nuclei, is used in the current context to apply specifically to the interaction of neutrons with nuclei, the consequent reaction type and resulting products.

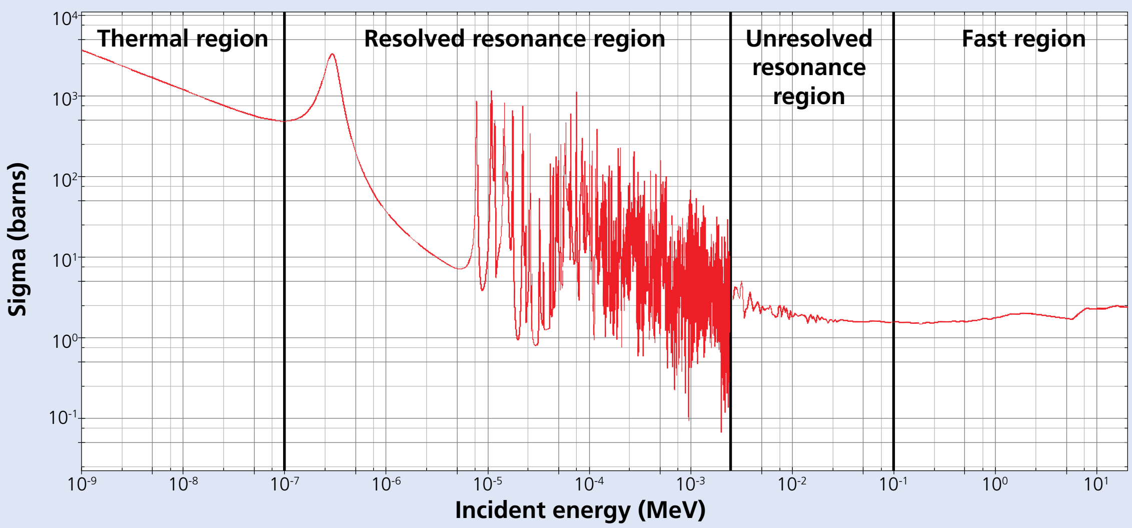
Neutron cross-sections

A fundamental concept for any consideration of particle interaction with matter is the cross-section, which is an expression of the likelihood that a reaction will take place. In the classical limit of an effectively zero sized particle interacting with a nucleus, the likelihood of interaction is represented by the cross-sectional area of the nucleus, πR^2 where R is the nuclear radius. The correct quantum mechanical description of the process is however, much more complex and the cross-section can be many orders of magnitude greater or smaller than πR^2. The total interaction cross-section is the sum of a number of partial cross-sections as described in Box 1.

The distinctive nature of the neutron-induced fission cross-section of plutonium-239 (^{239}Pu) is shown in Figure 1. At thermal energies the cross-section shows the normal $1/v$ behaviour for reaction cross-sections, where v is the neutron velocity. In the energy range of a few electron volts (eV) to several kilo electron volts (keV), the cross-section displays a resonant structure where the energy available to the absorbed neutron coincides with energy levels of the compound neutron-plus-nucleus system. This reaction mechanism persists into the unresolved resonance region but here the levels of the compound system are either too finely spaced to show distinct structure, or are unable to be resolved experimentally. In the fast region the resonance structure has disappeared and only slowly varying gross features are apparent.

Neutron cross-sections are used by neutronics modelling codes principally to solve the Boltzmann transport equation for the system angular neutron flux, as described in Box 2. This flux solution can be obtained either by Monte Carlo methods, where individual neutrons are tracked through the

FIGURE 1



The evaluated neutron-induced fission cross-section of ^{239}Pu, plotted logarithmically, from thermal energies up to 20 MeV (million electron volts). The energy boundaries of the regions defined in the figure are normally set by the evaluator.

BOX 1

Neutron interaction cross-sections

The likelihood that an incident neutron will react with a target nucleus is described by the 'total' cross-section and is denoted σ(total). In the following expression the total cross-section is represented as the sum of 'partial' cross-sections, each one of which represents the likelihood of a specific reaction:

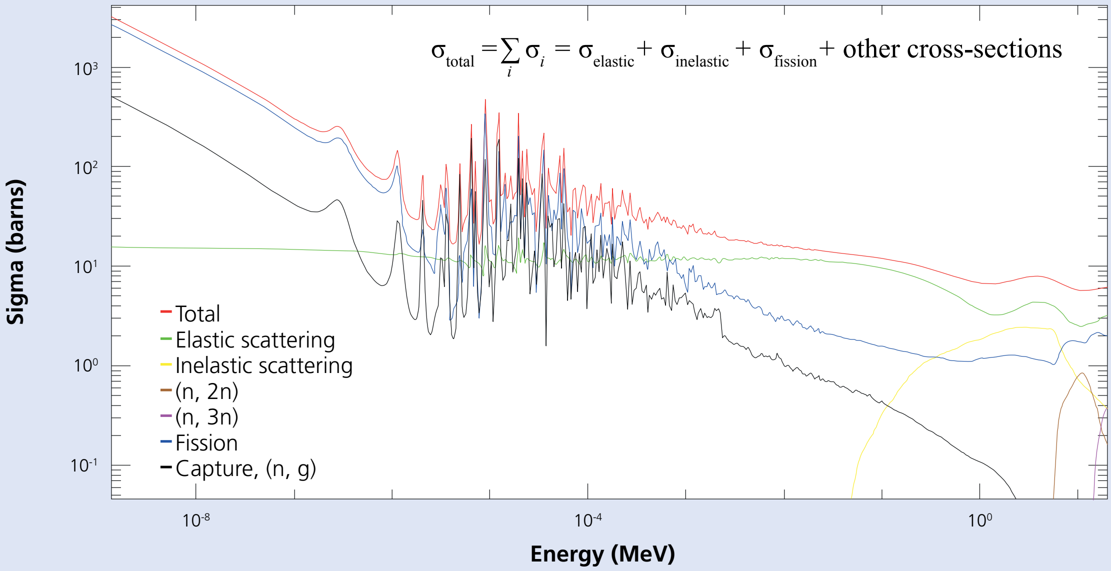
$$\sigma(\text{total}) = \sigma(\text{elastic}) + \sigma(\text{gamma}) + [\ \sigma(\text{inelastic}) + \sigma(\text{neutrons}) + \sigma(\text{fission}) + \text{other cross-sections}]$$

where the partial cross-sections are:

- σ(elastic) = elastic scattering (1 neutron emitted)
- σ(gamma) = capture reaction (gamma ray emission)
- σ(inelastic) = inelastic scattering (1 neutron + gamma ray emission)
- σ(neutrons) = more than 1 neutron + gamma ray emission
- σ(fission) = fission reaction (neutrons + fission products + gamma rays)

The elastic and capture reactions are always energetically possible, however the cross-sections enclosed in the square brackets denote that the reaction will only take place if the incoming neutron is above a certain threshold energy. In addition, the fission reaction will clearly only occur if the nucleus is *fissionable*; nuclides such as ^{235}U have a zero threshold for fission and are termed *fissile*. A set of cross-sections for neutrons interacting with ^{235}U is shown in Figure 2.

FIGURE 2



The total cross-section and partial cross-sections of ^{235}U from thermal energies to 20 MeV. Cross-sections have units of area and are measured in barns, where 1 barn = 10^{-24} cm^2.

system under study and their interaction histories recorded, or by discretising in time, energy, space and angle and solving the transport equation iteratively, as a deterministic problem.

Data sources

Cross-section data are collated and evaluated at a network of 14 data centres worldwide. Physicists at these centres assess the available data for a nuclide, derived from experiment and/or theory, and produce a recommended set of data. This evaluation is a subjective process, hence evaluations differ from centre to centre.

The three major evaluation projects are: JEFF (Joint Evaluated Fission and Fusion) based in Europe, ENDF (Evaluated Nuclear Data File) based in the US and JENDL, the Japanese Evaluated Nuclear Data Library.

NJOY processing

Nuclear data in its evaluated form cannot easily be used directly; processing into a friendlier and more accessible form is therefore required. The NJOY code is an internationally recognised standard [1] for undertaking this task; data can be cast into both continuous format for Monte Carlo applications, or group format for deterministic code applications.

Using NJOY requires specialised knowledge and skills. In recent years Serco Assurance have performed the necessary data processing for AWE, delivering data for a wide range of nuclides from the most up-to-date JEFF, ENDF and JENDL evaluations. These data are in a specialised group format called GENDF (Group ENDF), on a high fidelity 460 energy group grid.

Data validation

The GENDF files must be checked and validated by the Nuclear Data Team to ensure the data are fit for purpose; this validation is performed through application of a code called NDval (see Box 3). The data are then converted to AWE's format and benchmarked against standard systems. These take the form of critical assemblies and device models chosen from standard benchmark suites. If the data adequately reproduce the expected results – experimental values in the case of critical assemblies and previous calculations in the case of device models – then they are considered acceptable for use in modelling codes.

> "AWE has the capability to perform its own theoretical neutron cross-section calculations, through the use of publicly available and in-house modelling codes."

Data adjustment and comprehensive libraries

Constraints imposed by calculation time and memory usage mean that fine group data are rarely used in mainstream calculations; consequently, a set of production libraries must be created in a range of coarse group structures. For example, one dimensional (1D) models would generally be calculated using a standard 105 group structure, whereas for 3D models, 32 groups or fewer would be more appropriate.

Data adjustment is required to compensate for loss of accuracy when group structures are coarsened or when approximations are applied in neutronics transport algorithms; libraries are therefore produced in a variety of combinations of group structures and transport approximations. The data adjusted are the principal partial cross-sections of the nuclides ^{239}Pu, ^{235}U and ^{238}U. The adjustment procedure uses the AWE code NDxadj to vary selected cross-sections in broad energy regions such that a best fit is obtained to a set of standard benchmark systems.

To produce the final working or comprehensive libraries the code NDLI is used to apply any adjustments, condense the data and add specialised cross-section datasets, such as radiochemical tracers.

BOX 2

Neutron transport equation

The time dependent Boltzmann transport equation in energy group form can be expressed as:

$$\frac{1}{v_g}\left(\frac{\partial \o_g(\underline{r}, \underline{\Omega}, t)}{\partial t}\right) + \underline{\Omega} \cdot \underline{\nabla} \o_g(\underline{r}, \underline{\Omega}, t) + \sigma_g(\underline{r}) \o_g(\underline{r}, \underline{\Omega}, t) = \sum_{g'=1}^{g'=G} \int \beta_{g'g}(\underline{r}, \underline{\Omega}' \rightarrow \underline{\Omega})\, \o_{g'}(\underline{r}, \underline{\Omega}, t) d\underline{\Omega}' + S_g(\underline{r})$$

where the summation in the first term on the right hand side extends over G groups.

$\o_g(\underline{r}, \underline{\Omega}, t)$ is the angular flux in neutron energy group g, at a time t, in unit solid angle about a direction $\underline{\Omega}$, at a point with position vector $\underline{r}$.

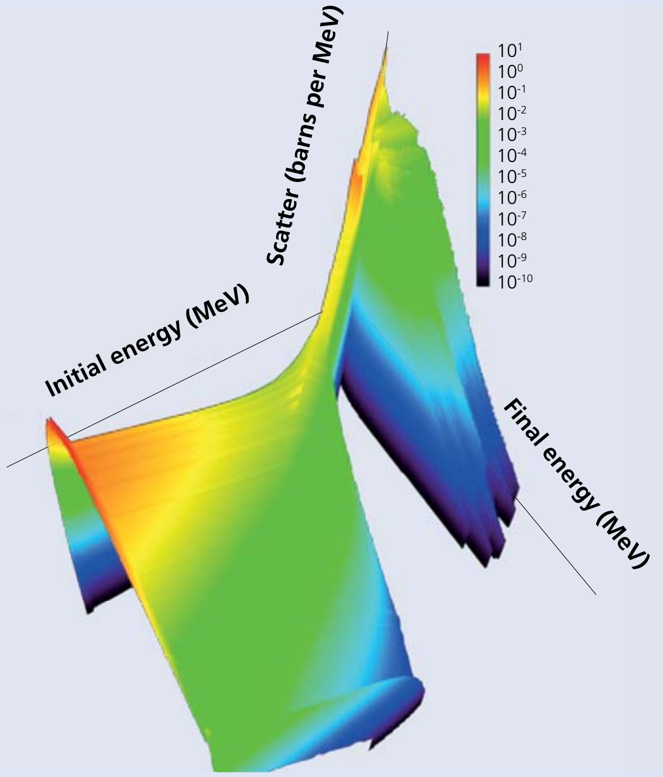
$\sigma_g(\underline{r})$ is the macroscopic total cross-section.

$\beta_{g'g}(\underline{r}, \underline{\Omega}' \rightarrow \underline{\Omega})$ is the transfer matrix (scatter + fission) which represents the scatter of neutrons in energy group g′, position $\underline{r}$ and direction $\underline{\Omega}'$ to energy group g, position $\underline{r}$ and direction $\underline{\Omega}$.

v_g is the velocity and $S_g(\underline{r})$ is a source term.

The main task of the Nuclear Data team is to provide the best available values for the quantities $\sigma_g(\underline{r})$ and $\beta_{g'g}(\underline{r}, \underline{\Omega}' \rightarrow \underline{\Omega})$. An example of the total cross-section has been shown in Box 1; an example of a transfer matrix is shown in Figure 3.

FIGURE 3



Example of a transfer matrix generated by the 3D graphics code NDview, showing the β scatter matrix for lithium-6 (^{6}Li) at a high temperature. At high initial energies the secondary distributions for threshold reactions, (i.e. inelastic scatter, (n, 2n), etc.), are visible. As the incident neutron energy decreases, the secondary distribution broadens indicating the enhanced upward and downward scatter due to thermal motion of the ^{6}Li nuclei. Energy scale in MeV decreases away from the origin.

BOX 3

Nuclear data codes

Specialised software has been developed over a number of years by AWE to process, manipulate and graphically display nuclear data. These codes have been developed, maintained and quality tested with the help of professional software consultants.

The main AWE codes are:

NDval: for validating the nuclear data produced in GENDF format by NJOY. A set of tests is applied to identify unphysical features or inconsistencies in the data.

NDconv: for conversion of data between different formats; in particular the conversion from NJOY generated GENDF format to AWE format.

NDxadj: for computing adjustments to data where necessary. The code iteratively compares calculated and experimental values of integral quantities such as critical assembly $k_{effective(s)}$ and produces a set of adjustments to provide the best fit.

NDLI: for applying adjustments if required, condensing to coarser group structures and combining libraries to create production libraries for use with AWE's modelling codes.

NDview: for graphical display of the data in 2D or 3D form. The code can read multiple formats and can perform a variety of operations on the data.

Benchmarking

Benchmarking is the definitive validation process for nuclear data and involves a comparison of results obtained through simulation with those obtained through experiment. This process is often employed during the release phase of a new nuclear data library as a method of verification and validation, and provides the end user with confidence that the data is consistent with physical quantities. Sensitivity studies may also be performed to provide a comparison between evaluated nuclear data libraries.

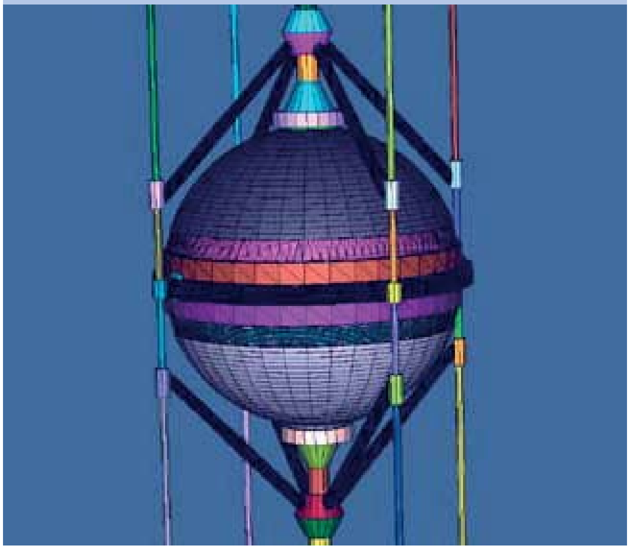
1D, 2D or 3D simulations are performed using a suitable neutronic modelling code and the results compared with a suite of experimental measurements. System eigenvalues such as $k_{effective}$ (a measure of system criticality) are often estimated as part of the validation process in addition to reactions rates, emission spectra and particle time of flight.

During benchmarking, it is important that the suite provides sufficient coverage of fissile materials, reflecting and moderating materials, neutron energies and material phases. This requirement is fulfilled by selecting a range of experimental systems including, bare/reflected fissile critical assemblies and high energy pulsed neutron systems.

ICSBEP provides an annual handbook containing benchmark specifications for experiments performed at various nuclear criticality facilities around the world [2]. The 'Jezebel' critical assembly was a near spherical, unreflected (i.e. bare), *δ-phase* ^{239}Pu experiment, operated throughout the 1950s at the Los Alamos National Laboratory (LANL). Designed to have minimal neutron reflection and highly reproducible results, many measurements were recorded including analytical eigenvalues ($k_{effective}$), neutron leakage spectra, and fission/activation reaction rates. Jezebel is considered to be one of the many experiments acceptable for use as a benchmark and features as one of the ICSBEP systems.

Neutronic modelling codes such as the LANL Monte Carlo Neutral Particle code – MCNP5 [3] – are often used to estimate integral quantities for critical or pulsed neutronic systems. A 3D model of Jezebel has been created at LANL using the MCNP5 code. Comparison of results obtained via simulation and experiment using three of the major nuclear

FIGURE 4



Plutonium-239 'Jezebel' Critical Assembly – complete.

FIGURE 5

Plutonium-239 'Jezebel' Critical Assembly – hemisphere.

data libraries are given in Tables 1 and 2. The complex geometry associated with the Jezebel critical assembly is illustrated in the 3D visualisations provided in Figures 4 and 5.

The LINDA library and data assessment

In the past, comprehensive libraries derived from the JEFF, ENDF and JENDL evaluations have been made available for use with AWE's modelling codes. The data in these libraries differ and can produce significantly different results when applied to the same problem. While it is useful to have these 'independent' libraries, for comparison with US and European collaborators for example, a proposal was made in 2008 to select the most suitable data for individual nuclides chosen from the major evaluations, based on the findings of physics based assessments.

The Library of Individual Nuclide Data Assessments (LINDA) is AWE's answer to this requirement and are the data recommended for use in design calculations.

Nuclear reaction theory

Nuclear physics is one area of science in which theory still trails experiment. However, theoretical calculations of nuclear data quantities are still necessary in regimes not accessible to experiment, for example nucleons incident on a nucleus in a short term excited (i.e. metastable) state. AWE has the capability to perform its own theoretical neutron cross-section calculations, through the use of publicly available [4-6] and in-house modelling codes.

TABLE 1

Experiment	1.0000 ± 0.0020	
	$k_{effective}$	$\pm 1\sigma$
ENDF/B-VII	0.9986	0.0001
JEFF 3.1	0.9986	0.0001
JENDL 3.2	0.9964	0.0001

Plutonium-239 'Jezebel' $k_{effective}$ values.

TABLE 2

	$\sigma_f\,(^{238}U)/\sigma_f\,(^{235}U)$ Calc/Exp	$\sigma_f\,(^{233}U)/\sigma_f\,(^{235}U)$ Calc/Exp	$\sigma_f\,(^{237}Np)/\sigma_f\,(^{235}U)$ Calc/Exp	$\sigma_f\,(^{239}Pu)/\sigma_f\,(^{235}U)$ Calc/Exp
ENDF/B-VII	0.9673	0.9862	0.9830	0.9738
JEFF 3.1	0.9915	0.9980	1.0043	0.9832
JENDL 3.2	0.9833	1.0042	0.9751	0.9716

Central fission rates table.

Unfortunately, there is no 'one size fits all' nuclear theory and different theoretical models are required to cover different mass and energy regimes. Although many of the codes available are able to automatically select an appropriate model to use, an experienced operator is nevertheless essential in ensuring not only that the correct model is chosen, but also that the right choices of input and library parameters are made.

One nuclear model which is applicable to a large proportion of calculations is the Optical Model [7]. In this approach, the complicated potential energy field created by the nucleons within a target nucleus is approximated as a single mean field potential. A neutron incident on this nucleus will then only interact with a single potential, thereby simplifying the calculation substantially.

If this mean field potential contains both real and imaginary terms, the incident neutrons may undergo reactions into either an elastic or a non-elastic channel (covering all reactions other than elastic scatter). Other nuclear models may then be used to calculate the proportion of neutrons in the non-elastic channel which undergo each individual reaction type, for example (n, 2n), (n, inelastic).

For nuclear reactions involving low energy neutrons and/or low mass nuclei, the *R*-matrix [8] approach is favoured due to the presence of resolved resonances in these regimes. These resonances are difficult to predict using other theories, and if measured data are available their parameters may be used to better tune the theoretical *R*-matrix model.

The main use for AWE's theoretical capability is to assist in the validation of imported cross-section data and make informed choices about which datasets to select for LINDA, but it can also be used to generate data for nuclei where none currently exist.

Nuclear data uncertainties and their propagation in calculations

Neutron cross-sections, like any other physical quantity have an uncertainty associated with their true value. For experimentally derived data this uncertainty is due to measurement error while, for data calculated from theory, it arises from uncertainties in the parameters used in the modelling code.

As the nuclear data available within AWE's libraries are generally in group format, uncertainties are specified for the average cross-section of each energy group. This makes it especially convenient when taking into account 'covariance' (i.e. the correlation between the uncertainties in two different groups).

Covariance arises due to the fact that, in general, experiments to determine a cross-section at one energy are not independent of measurements made at a different energy. For example, a particular detector may produce a systematic error that extends over an energy range bridging several energy groups, leading to correlated uncertainties in the measured cross-sections in adjacent groups.

The covariance of two quantities, x_1 and x_2, is analogous to the variance of a single quantity, and may be written mathematically as:

$$\mathrm{cov}(x_1, x_2) = \sum_{i=1}^{n} \frac{(x_{1_i} - \bar{x}_1)(x_{2_i} - \bar{x}_2)}{n}$$

where, n is the number of measurements made of x_1 and x_2. The covariances in all of the energy groups for a cross-section may be stored conveniently in a covariance matrix, V_x:

$$V_x = \begin{pmatrix} \mathrm{var}(x_1) & \mathrm{cov}(x_1,x_2) & \dots & \mathrm{cov}(x_1,x_n) \\ \mathrm{cov}(x_2,x_1) & \mathrm{var}(x_2) & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \mathrm{var}(x_n) \end{pmatrix}$$

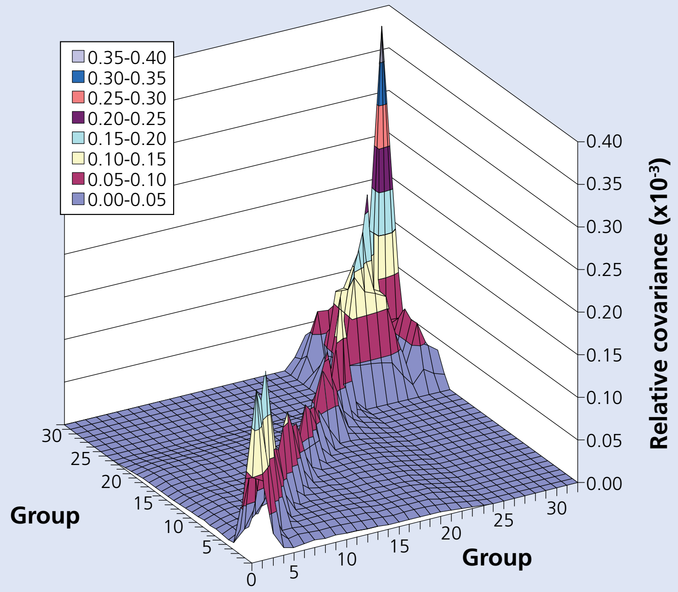
where the diagonal terms are the variances and the off diagonal terms are the covariances between the measured quantities. It is often easier to visualise these matrices in 3D plots as shown in Figure 6.

The uncertainty in the nuclear data used in a calculation will lead to an uncertainty in the value of any quantity calculated using it. Covariance data can be used to calculate this uncertainty via the 'Sandwich Equation':

$$\sigma_y = \sqrt{\underline{D}^T \, \underline{V}_x \, \underline{D}}$$

where D and D^T are a vector of 'sensitivity coefficients' and its transpose respectively, and σ_y is the uncertainty (or standard

FIGURE 6



Plutonium-239 (n,f) relative covariance data from the ENDF/B-VII evaluation.

deviation) of some integral quantity which is the desired output of the calculation. These sensitivity coefficients are simply the rate of change of the integral parameter of interest with respect to cross-section for a particular energy group.

Covariance data from the ENDF/B-VII library have been used to successfully calculate the uncertainty of $k_{effective}$ for AWE's suite of critical assembly benchmarks [9]. The results of a subset of uranium benchmarks are given in Table 3 and show that in each case the uncertainty from propagated data errors exceeds the uncertainty from experiment.

Future work

LINDA is an evolving project and when significant new evaluations become available, the data will be assessed and, if deemed suitable, will be included in future library releases. NJOY processing skills are being developed to enable an in-house capability for future data acquisition.

Our data adjustment capability is being extended to include the use of data available from a wider range of experimental systems. To date only spherical (i.e. 1D) systems taken from the ICSBEP compilation have been used; a capability to include 2D systems has recently been implemented in NDxadj.

In the 1970s the Lawrence Livermore National Laboratory in the US undertook a programme of experiments measuring the neutron spectra produced when a wide variety of materials was bombarded with 14 MeV neutrons. These data give important information on neutron cross-sections at high energy; methods will be developed to exploit this experimental data, both for benchmarking and adjustment purposes.

Data uncertainty studies will be extended to cover more general non-linear cases where the use of the 'Sandwich Equation' may no longer be valid.

Although this article relates mainly to nuclear data activities in connection with neutron transport through materials, neutron interaction cross-sections are also used to modify the system nuclide inventory through transmutation reactions. An ongoing important and challenging task for AWE is to provide reliable cross-section sets, particularly for radiochemistry interpretation, which plays a pivotal role in its modelling capability.

TABLE 3

Sample	Reflector material	Thickness (cm)	Calculated uncertainty (%)	Experimental uncertainty (%)
1	Uranium	20.32	0.3993	0.3000
2	Polyethylene	1.45	0.3599	0.2800
3	Steel	9.70	0.3031	0.2400
4	Beryllium	4.70	0.3216	0.3000

Comparison of theoretical and experimental $k_{effective}$ percentage uncertainties for some uranium benchmarks.

References

[1] R.E. MacFarlane, D.W. Muir, The NJOY nuclear data processing system, LA- 12740-M (1994).

[2] J.B. Briggs *et al.*, International handbook of evaluated criticality safety benchmark experiments, NEA/NSC/DOC(95)04/I, Nuclear Energy Agency, France (2004).

[3] X-5 Monte Carlo Team, MCNP - A general Monte Carlo N-Particle Transport Code, Version 5, Los Alamos National Laboratory, LA-UR-03-1987 (2003).

[4] P.G. Young, E.D. Arthur, Proceedings of Computation and Analysis of Nuclear Data Relevant to Nuclear Energy and Safety, Trieste, Italy (1992).

[5] M. Herman, Proceedings of Workshop on Nuclear Reaction Data and Nuclear Reactors: Physics, Design and Safety, Trieste, Italy (2000).

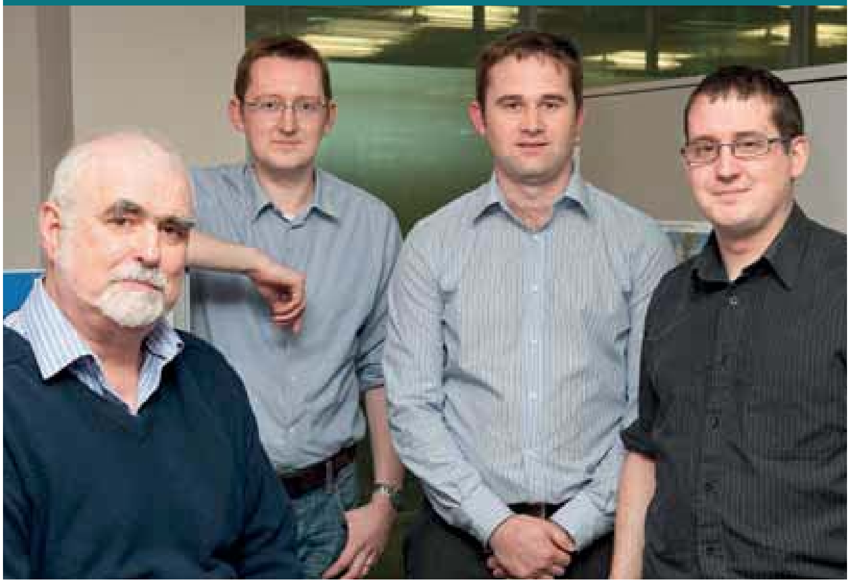
[6] A.J. Koning, S. Hilaire, M.C. Duijvestijn, TALYS-1.0, Proceedings of the International Conference on Nuclear Data for Science and Technology, Nice, France (2007).

[7] A.J. Koning, J.P. Delaroche, Local and global nucleon optical models for 1 keV to 200 keV, Nucl. Phys. A 713, 231 (2003).

[8] A.M. Lane, R.G. Thomas, R-Matrix theory of nuclear reactions, Rev. Mod. Phys. 30, 257 (1958).

[9] J. Benstead, Nuclear data uncertainty propagation through a critical assembly benchmark suite, Proceedings of the International Conference on Mathematics and Computational Methods Applied to Nuclear Science and Engineering, Brazil (2011).

AUTHOR PROFILE



Left to right, Bruce Thom (Team Leader), James Benstead, Mark Jackson and Mark Cornock.

Bruce Thom

Bruce graduated from Edinburgh University with an honours degree in Physics in 1972 after which he moved to Queen Mary College in London to study for a PhD. He joined AWE in 1993 since when he has been principally responsible for the provision of nuclear data for AWE's modelling codes.

James Benstead

James graduated from the University of Lancaster with an MPhys (1st Class Honours). James joined AWE in 2006 and is currently undertaking a sponsored collaborative PhD at the University of Surrey studying the theoretical calculation of neutron interaction cross-sections.

Mark Jackson

Mark graduated from University College London with a BSc (1st Class Honours) in Physics. In 2007 he joined AWE and is currently working on the testing and benchmarking of nuclear data.

Mark Cornock

Mark joined AWE in 2006 after graduating with an MPhys in Physics with Planetary and Space Physics from the University of Wales. Since joining AWE Mark has principally been involved in the production and validation of nuclear data libraries.

Research into Information Barrier Systems